

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 368 °C

Global applicability domain: Inside

Local applicability domain index: 2.48e-01

Confidence level: 4.60e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Benzenemethanol, .alpha.,.alpha.-diphenyl-</div> <div>Measured: 380</div> <div>Predicted: 348</div>	<div>Image not found</div> <div>Benzoin</div> <div>Measured: 344</div> <div>Predicted: 319</div>	<div>Image not found</div> <div>Benzoin</div> <div>Measured: 344</div> <div>Predicted: 319</div>
<div>Image not found</div> <div>4-Cumylphenol</div> <div>Measured: 335</div> <div>Predicted: 317</div>	<div>Image not found</div> <div>Hexachlorophene</div> <div>Measured: 479</div> <div>Predicted: 416</div>	